A Strategy for Simulation of Long Term Fuel Storage and Subsequent Transport

G. Hansen, S. Novascone, R. Williamson

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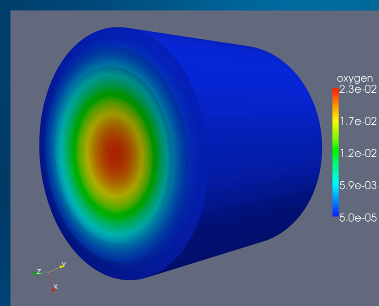

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Fuel lifetime

Fuel Performance
- Hydrogen uptake
- Cladding abuse (fretting)

Drying
- Hydride reorientation
- Thermal soak
- High stresses

Long term storage
- Corrosion (?)
- Creep (?)
- Fuel oxidation (?)

Transport
- Low cycle fatigue
- Fracture toughness

Off-normal events
- Accidents
- Drop simulation

- Fuel performance calculation is the basis for cladding stress state on entry to drying cycle
- Not sure what the relevant physics is across the cycle
  - Rapid “plug and play” model replacement to support exploration of various effects
  - Sensitivity analysis
- How does longer burnup effect aging?
- How do all these uncertainties add up?

Simulation can answer many questions

- Easily look at the complete cycle, different fuel and reactor types, different operational conditions (longer burnup)
- Readily build intuition and test relative importance of different phenomena
- Employ implicit integration to allow 100 year storage periods to be computed with only a few time steps.
- Get results quickly and relatively inexpensively.
- Track predictions and address unexpected issues in long term tests

Assist with analytically closing the gaps.

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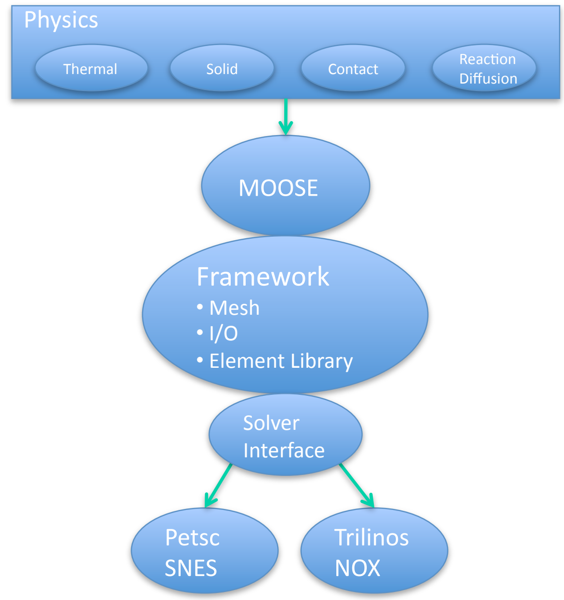
Simulation strategy

- Develop simulation basis for long term storage and subsequent transport
- Fuel performance code sets initial conditions for drying
- Drying process modeled with same code, using hydride and thermomechanical models in cladding (fuel still present for PCI).
- Storage period may include corrosion (inside the fuel) and cladding creep.
- Transport will include vibration, stress and strain, and low cycle fatigue in cladding

What capabilities can be leveraged to perform end-to-end calculations of this sort?

MOOSE: A coupled multiphysics framework

- Clean physics interface for ease of development of new applications
  - Physics Interface conceals framework complexity
- Framework provides core set of common services
  - libMesh: http://libmesh.sf.net
- 1D, 2D, and 3D; steady state and transient with same code
- Adaptive, parallel, fully coupled, fully implicit, portable
  - Robust solvers are key for “ease of use”
  - Load balancing and mesh adaptation are tightly integrated to form a robust “dial free” application



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MOOSE Ecosystem

Application	Physics	Start	Time To Results
BISON	Thermo-mechanics, Chemical Diffusion, coupled mesoscale	June 2008	4 Months
PRONGHORN	Neutronics, Porous Flow, Eigenvalue	September 2008	3 Months
SALMON	Multiphase Porous Flow	June 2009	3 Months
MARMOT	4th Order Phasefield Mesoscale	August 2009	1 Month
RAT	Porous ReActive Transport	August 2009	1 Month
FALCON	Geo-mechanics, coupled mesoscale	September 2009	3 Months

BISON – A MOOSE fuel performance code

- Transient, nonlinear heat conduction

$$\rho C_p T_t - \nabla \cdot k \nabla T - q = 0$$

- Nonlinear oxygen diffusion

$$s_t - \nabla \cdot (D(\nabla s + \frac{sQ^*}{FRT^2} \nabla T)) = 0$$

- Linear elastic model, nonlinear material properties

$$\begin{aligned}(u_{tt}, \phi) \quad &+ \quad \mu S(u,\phi) + \lambda(\nabla \cdot u, \nabla \cdot \phi) \\ &- \quad (f,\phi) - \langle g, \phi \rangle - (\alpha T, \nabla \phi) = 0\end{aligned}$$

$$S(u,\phi) = \sum_{i,j=1}^{3} (\partial_j u_i + \partial_i u_j)(\partial_j \phi_i + \partial_i \phi_j)$$

Additional physics currently in BISON

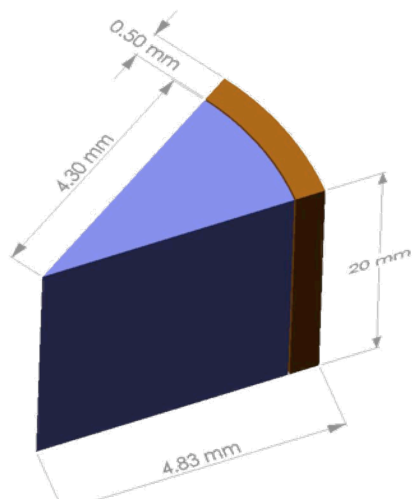
- Temperature and burnup dependent thermal properties of fuel
- Fission product swelling
  - Gas
  - Solid
- Burnup
- Fission gas release in progress
- Other closure relations

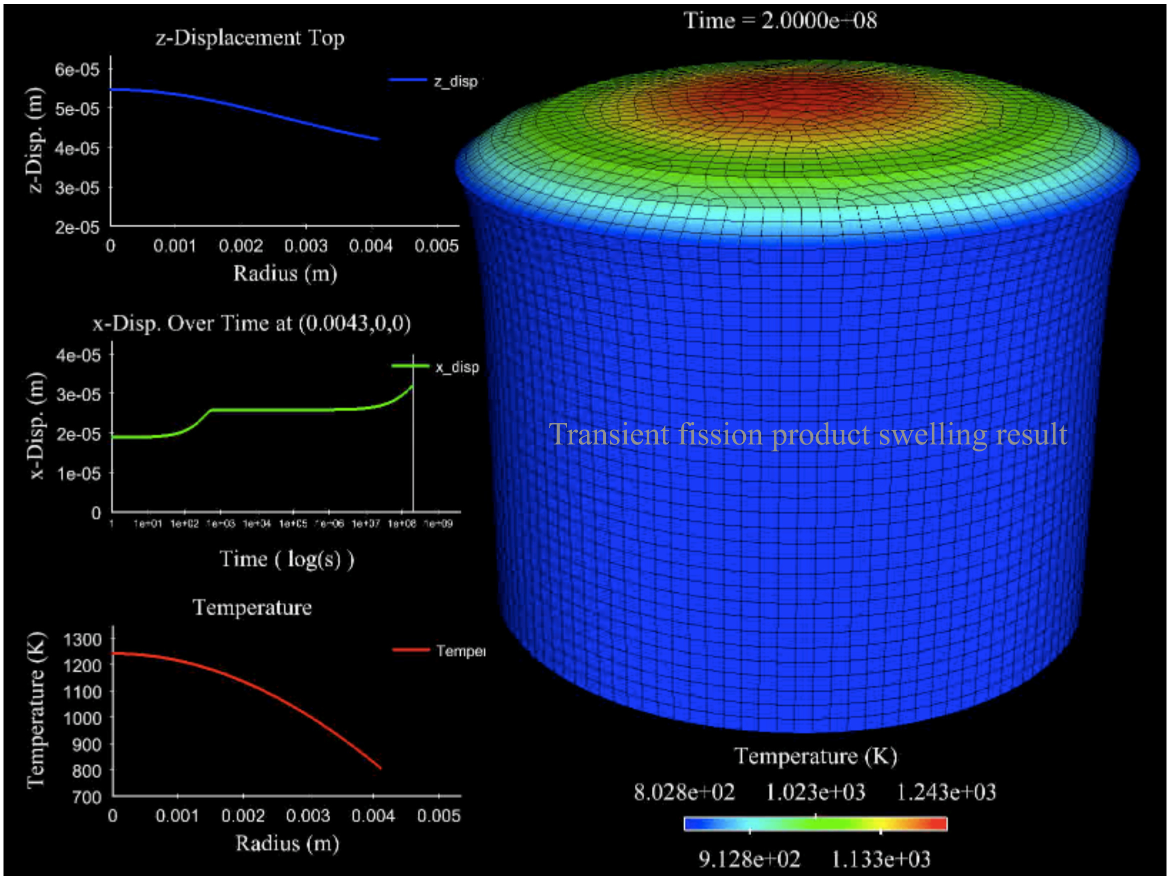
Potential Collaboration

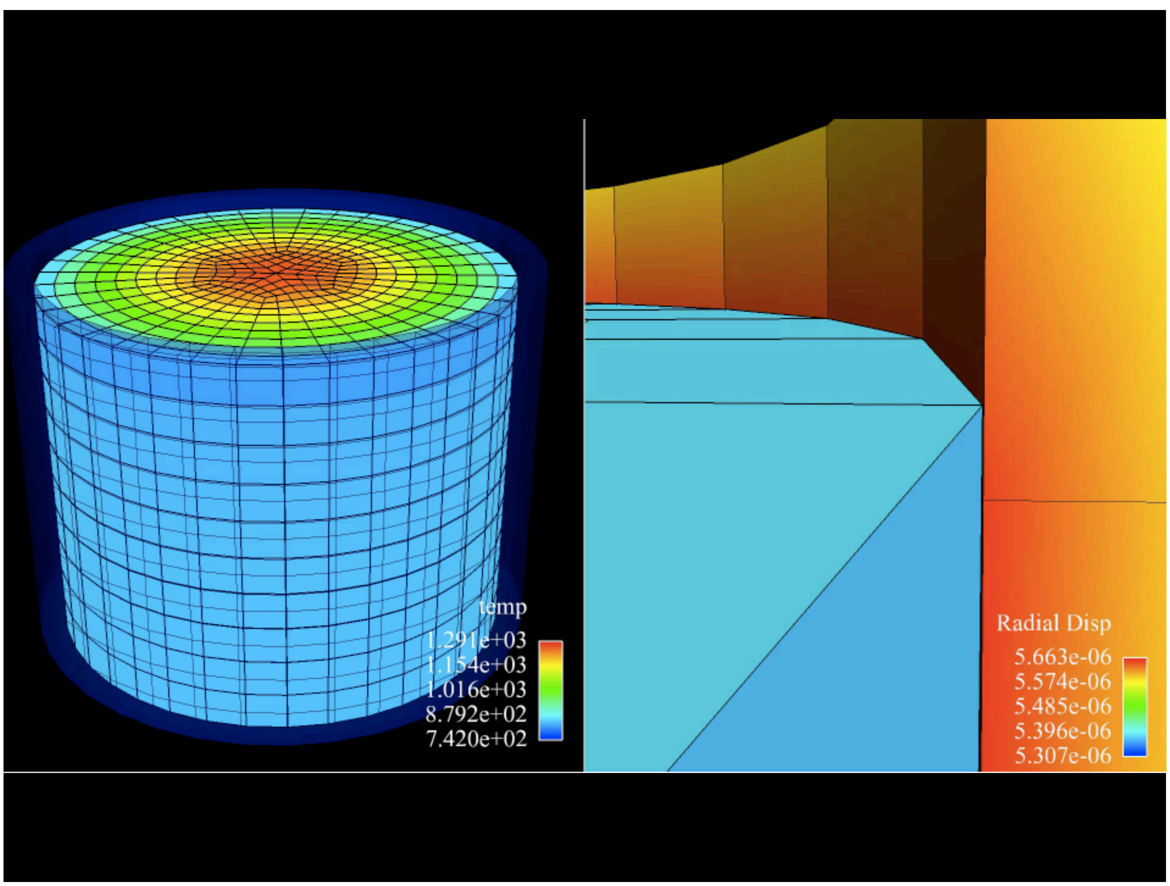
- ANATECH has expressed interest in active collaboration on MOOSE/BISON development
- Joe and Mark Rashid have done significant recent work in damage mechanics and hydride reorientation
- FALCON includes a spent fuel capability including post-irradiation cladding creep

Coupled thermomechanics & oxygen diffusion

- Extension of previous work of Ramirez, Stan, and Cristea, J. Nuclear Materials, 2006.
- Extended to 3D
- JFNK solution of fully coupled thermomechanics and oxygen diffusion



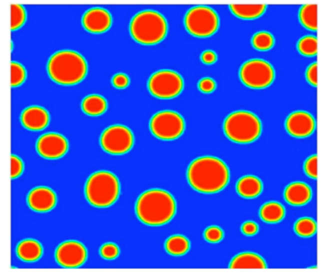

Time = 2.0000e+08
z-Displacement Top
z_disp
z-Disp. (m)
6e-05
5e-05
4e-05
3e-05
2e-05
0
0.001
0.002
0.003
0.004
0.005
Radius (m)
x-Disp. Over Time at (0.0043,0,0)
x_disp
x-Disp. (m)
4e-05
3e-05
2e-05
1e-05
0
Time (log(s))
Temperature
Temperature (K)
1300
1200
1100
1000
900
800
700
Radius (m)
Transient fission product swelling result
Temperature (K)
8.028e+02
1.023e+03
1.243e+03
9.128e+02
1.133e+03

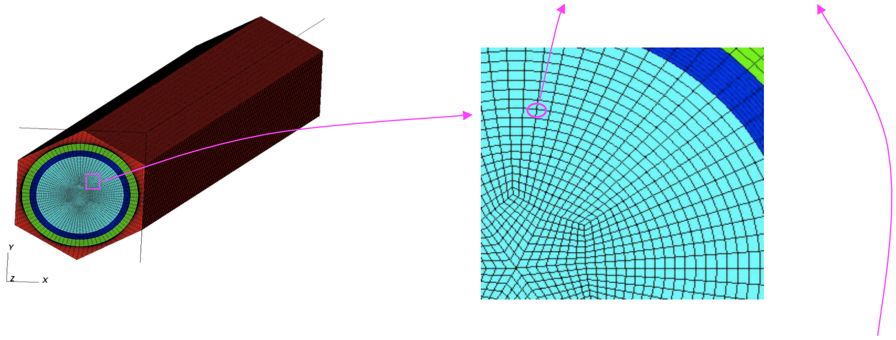

temp
1.291e+03
1.154e+03
1.016e+03
8.792e+02
7.420e+02
Radial Disp
5.663e-06
5.574e-06
5.485e-06
5.396e-06
5.307e-06

Fully-coupled bridging to/from mesoscale

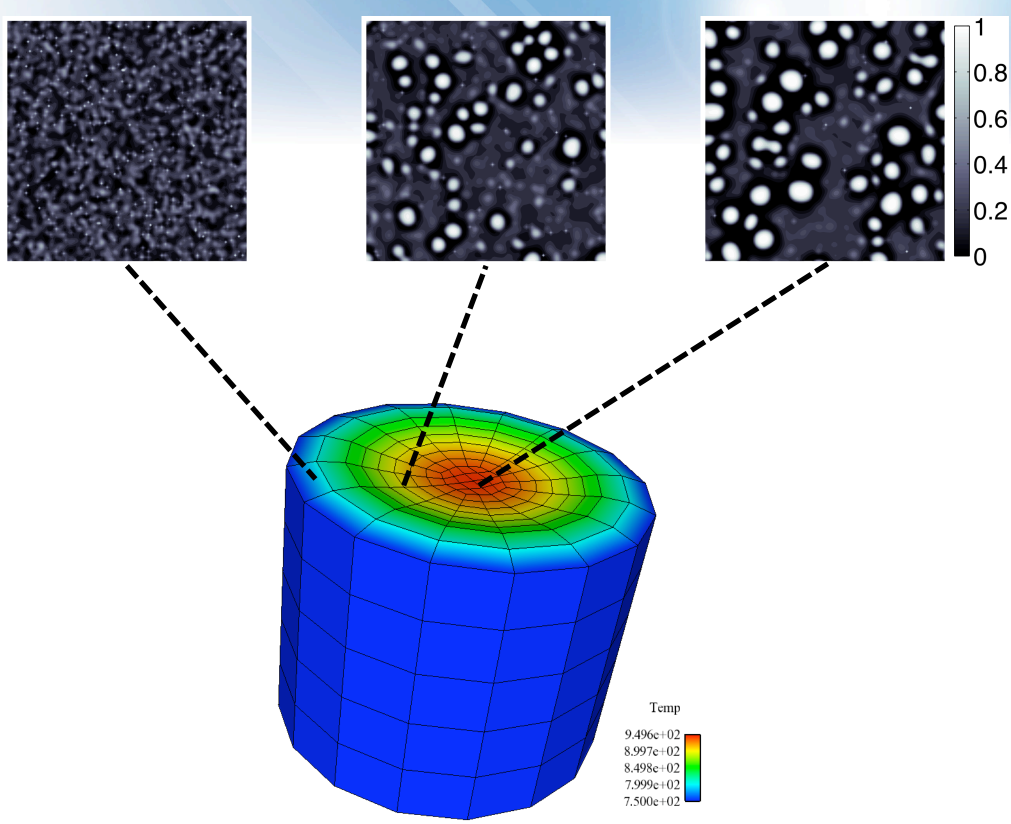
The energy equation is solved at the engineering scale for temperature using JFNK

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot q + \dot{Q}$$





S.K. Rokkam, P.C. Millett, D. Wolf, and A. El-Azab, "Phase Field Simulation of Void Growth in Irradiated Materials," Fourth International on Multiscale Materials Modeling, Symposium 4-Multiscale modeling of microstructure evolution in materials, Oct. 27-31, pages 405-408



Equation System

- All variables are solved simultaneously
  - Phase field residual equations

$$\mathbf{R}_{c_i} = \frac{\partial c_i}{\partial t} - \nabla \cdot \left(M_{ij} \nabla \left(\frac{\partial g_0}{\partial c_i} - \kappa \nabla^2 c_i + \frac{\partial E_{el}}{\partial c_i} \right) \right) = \mathbf{0} \qquad \mathbf{R}_{\eta_i} = \frac{\partial \eta_i(\mathrm{r},t)}{\partial t} + L_i \left(\frac{\partial f_0}{\partial \eta_i} - \kappa \nabla^2 \eta_i + \frac{\partial E_{el}}{\eta_i} \right) = \mathbf{0}$$

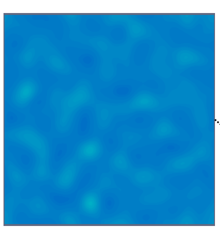
  - Coupled variable residual equations

$$\mathbf{R}_u = \nabla \cdot (\mathbf{C} \nabla \mathbf{u}) - \nabla \cdot (\mathbf{C} \varepsilon^*) = \mathbf{0}$$

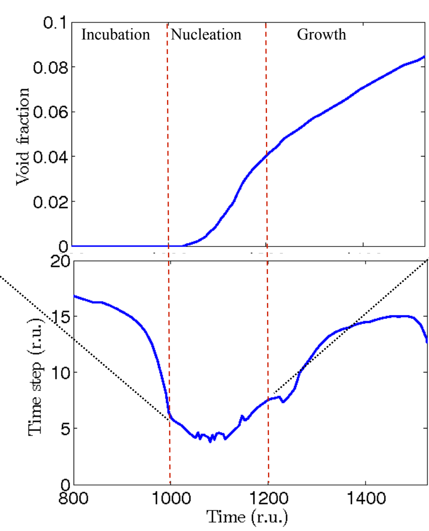
- FEM discretization

$c_i(\mathbf{r}) = \sum_{j=1}^{N} c_i^j \varphi_j(\mathbf{r})$	$\eta_i(\mathbf{r}) = \sum_{j=1}^{N} \eta_i^j \varphi_j(\mathbf{r})$	$\mathbf{u}(\mathbf{r}) = \sum_{j=1}^{N} \mathbf{u}^j \varphi_j(\mathbf{r})$
Discretized using 3rd order Hermite element	*Discretized using 1st order Lagrange elements*	*Discretized using 1st order Lagrange elements*
2D: 20 DOF	*2D: 8 DOF*	*2D: 8 DOF*
3D:36 DOF	*3D: 12 DOF*	*3D: 12 DOF*

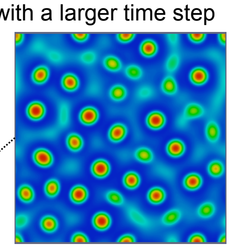
Adaptive Time Step



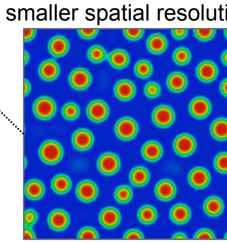
Void nucleation requires small spatial resolution



Void growth can be resolved with a larger time step

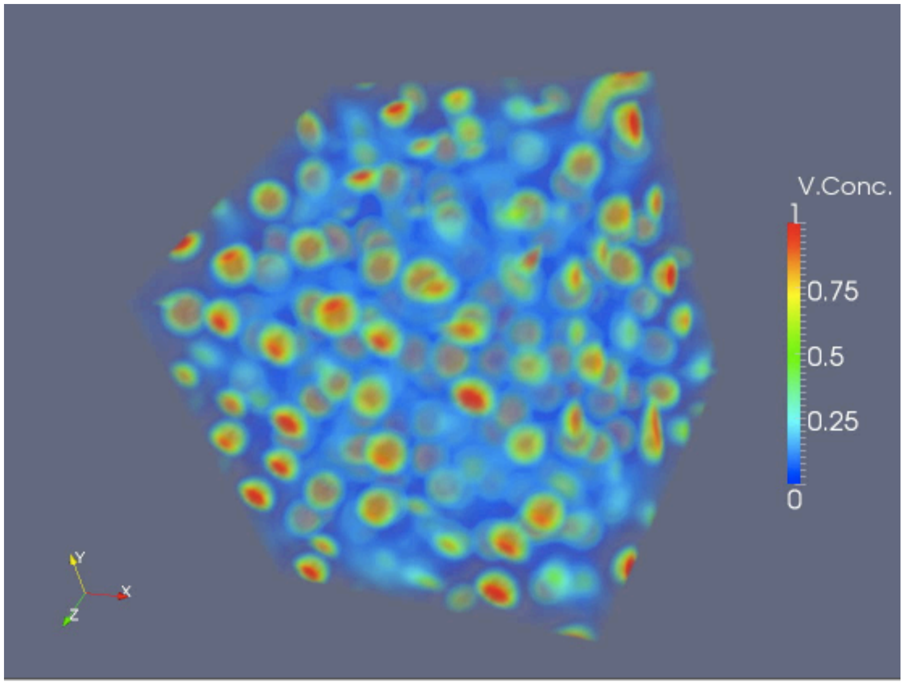


Void coalescence needs smaller spatial resolution



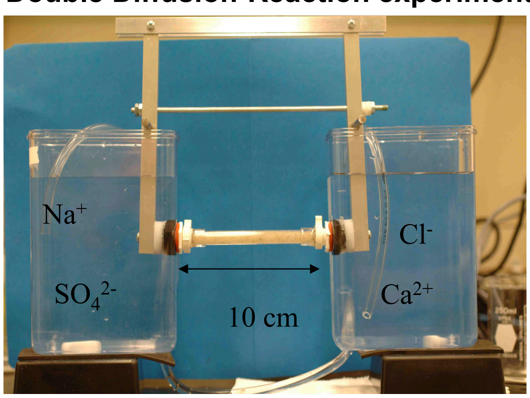
- Solution time step adapts to the driving phenomena

3-D Void Nucleation and Growth

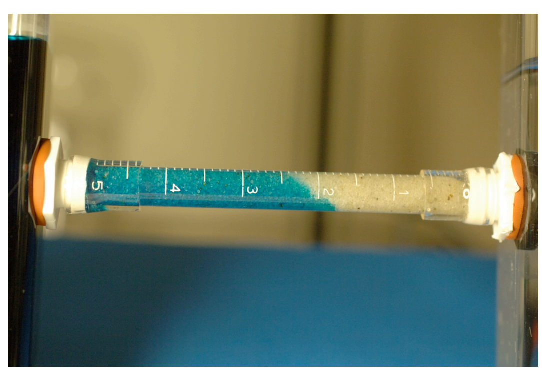


Modeling of coupled diffusion and mineral precipitation in porous media

Double Diffusion-Reaction experiment



Focused precipitation front – visible only by using dye



$$(1)\quad \frac{\partial\left[\theta\left(C_{Ca^{2+}}+C_{CaCl^{+}}+C_{CaCl_2(aq)}+C_{CaOH^{+}}+C_{CaSO_4(aq)}+C_{CaSO_4(s)}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{Ca^{2+}}+C_{CaCl^{+}}+C_{CaCl_2(aq)}+C_{CaOH^{+}}+C_{CaSO_4(aq)}\right)\right]=0$$

$$(2)\quad \frac{\partial\left[\theta\left(C_{Cl^-}+C_{CaCl^{+}}+2C_{CaCl_2(aq)}+C_{HCl(aq)}+C_{NaCl(aq)}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{Cl^-}+C_{CaCl^{+}}+2C_{CaCl_2(aq)}+C_{HCl(aq)}+C_{NaCl(aq)}\right)\right]=0$$

$$(3)\quad \frac{\partial\left[\theta\left(C_{H^+}+2C_{H_2SO_4(aq)}+C_{HCl(aq)}+C_{HSO_4^-}-C_{CaOH^+}-C_{NaOH(aq)}-C_{OH^-}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{H^+}+2C_{H_2SO_4(aq)}+C_{HCl(aq)}+C_{HSO_4^-}-C_{CaOH^+}-C_{NaOH(aq)}-C_{OH^-}\right)\right]=0$$

$$(4)\quad \frac{\partial\left[\theta\left(C_{Na^+}+C_{NaCl(aq)}+C_{NaOH(aq)}+C_{NaSO_4^-}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{Na^+}+C_{NaCl(aq)}+C_{NaOH(aq)}+C_{NaSO_4^-}\right)\right]=0$$

$$(5)\quad \frac{\partial\left[\theta\left(C_{SO_4^{2-}}+C_{CaSO_4(aq)}+C_{H_2SO_4(aq)}+C_{HSO_4^-}+C_{NaSO_4^-}+C_{CaSO_4(s)}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{SO_4^{2-}}+C_{CaSO_4(aq)}+C_{H_2SO_4(aq)}+C_{HSO_4^-}+C_{NaSO_4^-}\right)\right]=0$$

$$(6)\quad \frac{d\left(C_{CaSO_4(s)}\right)}{dt}-0.1\times 6.456542\times 10^{-8}\times\left(1-\frac{C_{Ca^{2+}}\cdot C_{SO_4^-}}{10^{-1.8487}}\right)=0$$

$$(7)\quad C_{CaCl^+}-10^{-0.7}C_{Ca^{2+}}\cdot C_{Cl^-}=0$$

$$(8)\quad C_{CaCl_2(aq)}-10^{-0.653}C_{Ca^{2+}}\cdot\left(C_{Cl^-}\right)^2=0$$

$$(9)\quad C_{CaOH^+}-10^{-12.85}C_{Ca^{2+}}\cdot\left(C_{H^+}\right)^{-1}=0$$

$$(10)\quad C_{CaSO_4(aq)}-10^{2.1}C_{Ca^{2+}}\cdot C_{SO_4^-}=0$$

$$(11)\quad C_{H_2SO_4(aq)}-10^{-1.021}\left(C_{H^+}\right)^2\cdot C_{SO_4^-}=0$$

$$(12)\quad C_{HCl(aq)}-10^{0.7}C_{H^+}\cdot C_{Cl^-}=0$$

$$(13)\quad C_{HSO_4^-}-10^{1.976}C_{H^+}\cdot C_{SO_4^-}=0$$

$$(14)\quad C_{NaCl(aq)}-10^{-0.782}C_{Na^+}\cdot C_{Cl^-}=0$$

$$(15)\quad C_{NaOH(aq)}-10^{-14.799}C_{Na^+}\cdot\left(C_{H^+}\right)^{-1}=0$$

$$(16)\quad C_{NaSO_4^-}-10^{0.82}C_{Na^+}\cdot C_{SO_4^-}=0$$

$$(17)\quad C_{OH^-}-10^{-13.991}\left(C_{H^+}\right)^{-1}=0$$

Challenges:

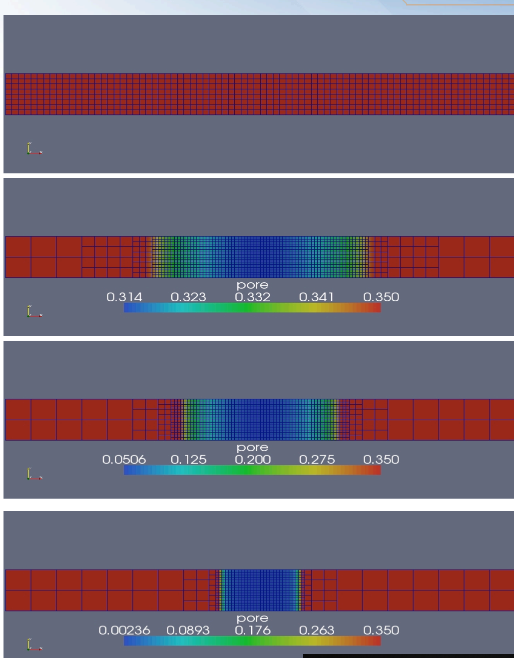
- **Both fast and slow kinetics**
- **Strongly coupled processes**

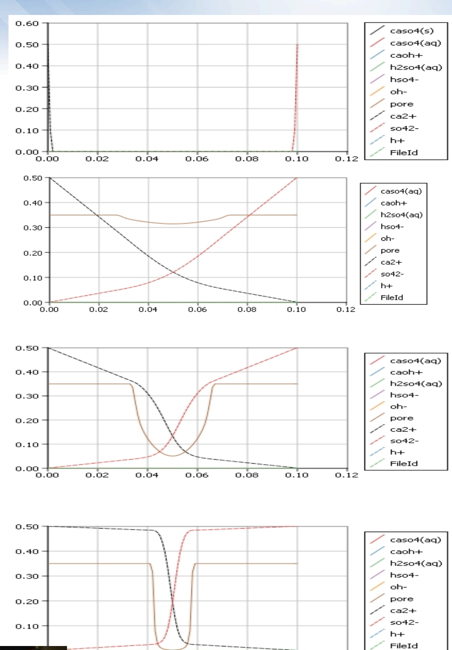
Conventional Approach:

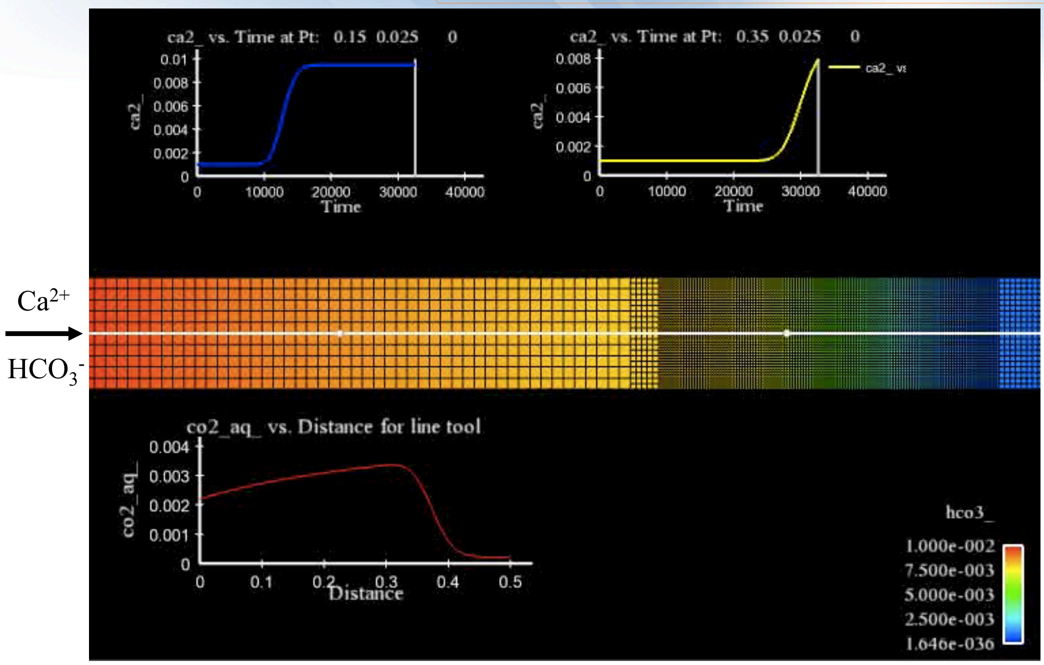
- **Operator splitting**

Our approach:

- **Fully coupled, fully implicit**
- **Adaptive mesh refinement**







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Concluding remarks

- The Multiphysics Object-Oriented Simulation Environment, MOOSE, supports rapid, 3-D, parallel, applications code development.
- MOOSE could readily be extended to incorporate the additional model sets that span the requirements for simulation of long term fuel storage and transport processes.